

Thermodynamic hierarchies of evolution equations

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Abstract. Non-equilibrium thermodynamics with internal variables introduces a natural hierarchical arrangement of evolution equations. Three examples are shown: a hierarchy of linear constitutive equations in thermodynamic rheology with a single internal variable, a hierarchy of wave equations in the theory of generalized continua with dual internal variables and a hierarchical arrangement of the Fourier equation in the theory of heat conduction with current multipliers.

Key words: multiscale, non-equilibrium thermodynamics, internal variables.

1. Introduction

Theories and material models of multiscale phenomena in space and time treat the scale changes either as a step from a micro- or mesoscopic statistical level to the phenomenological one or as a reduction of the degrees of freedom by averaging over a field variable or spatial dimension. The characteristic methodology is similar to the BBKGY hierarchy of the kinetic theory [1, 2]. In these approaches, the modeling of transitional effects requires the detailed knowledge or the drastic simplification of the material structure.

In this work, we show that a hierarchical arrangement of evolution equations is apparent in thermodynamics with internal variables where the different levels of the hierarchy are regulated by material parameters. The scale transitions are natural and dynamical.

We show three examples. First, a hierarchy of ordinary differential equations is presented in the thermodynamic rheology of solids with a single internal variable. The building block of the hierarchy is the basic constitutive equation of elasticity. This is a hierarchy between the different time scales of the evolution, a *time hierarchy*.

Then a hierarchy of hyperbolic partial differential equations is shown in the thermodynamic theory of generalized continua with dual internal variables. The building block of the hierarchy is the wave equation. This is a dynamic hierarchy between different time and length scales of the evolution, a *space-time hierarchy*.

Finally, a hierarchy of parabolic partial differential equations is shown in the thermodynamic theory of heat conduction with current multipliers. The building block of the hierarchy is the Fourier equation. Like the previous example, it is a dynamic hierarchy between different time and length scales of the evolution, a *space-time hierarchy*.

2. The hierarchy of rheological bodies and the Kluitenberg–Verhás model

In the thermodynamic approach to rheology, an extended state space is chosen, which is spanned by the following variables: specific internal energy e , strain ε , and an internal variable ξ . This modeling approach is well-known for fluids [3, 4, 5, 6, 7] and has been introduced recently for solids [8]. The internal variable is a second order symmetric tensor, based on our purpose to gain an extension of the mechanical aspects (the ‘material law’) of the initial system, to obtain corrections to the relation between stress and strain, which quantities are both symmetric tensors.

We shift entropy by a concave nonequilibrium term depending—quadratically—on ξ only. According to the Morse lemma, this new entropy term can be chosen as a pure square term, hence, the extended specific entropy function \tilde{s} is

$$\tilde{s}(e, \varepsilon, \xi) = s(e, \varepsilon) - \frac{1}{2} \text{tr}(\xi^2), \quad (1)$$

where tr denotes the trace of a second order tensor and we have denoted the classical specific entropy without tilde. The Gibbs relation for the extended entropy is a convenient particular thermodynamic notation for the partial derivatives, the intensive quantities:

$$\rho d\tilde{s} = \frac{\rho}{T} de - \frac{1}{T} \text{tr}(\sigma d\varepsilon) - \rho \text{tr}(\xi d\xi). \quad (2)$$

Here ρ is the density, T is the temperature and σ is the thermostatic stress. Stress is also considered extended by a rheological (nonequilibrium) term:

$$\tilde{\sigma} = \sigma + \hat{\sigma}. \quad (3)$$

Consequently, the mechanical power, and correspondingly the energy balance, gets shifted as

$$\rho \dot{e} + \nabla \cdot \mathbf{j}_e = \text{tr}(\tilde{\sigma} \dot{\varepsilon}) = \text{tr}(\sigma \dot{\varepsilon}) + \text{tr}(\hat{\sigma} \dot{\varepsilon}). \quad (4)$$

Here \mathbf{j}_e is conductive current density of the internal energy, the heat flux. With the choice $\mathbf{j}_{\tilde{s}} = \mathbf{j}_e/T$, and utilizing (2) and (4), the entropy production is found to be

$$\begin{aligned} \Sigma &= \rho \dot{\tilde{s}} + \nabla \cdot \mathbf{j}_{\tilde{s}} = \frac{\rho}{T} \dot{e} - \frac{1}{T} \text{tr}(\sigma \dot{\varepsilon}) - \rho \text{tr}(\xi \dot{\xi}) + \nabla \cdot \left(\frac{\mathbf{j}_e}{T} \right) \\ &= -\frac{1}{T} \nabla \cdot \mathbf{j}_e + \frac{1}{T} \text{tr}(\hat{\sigma} \dot{\varepsilon}) - \rho \text{tr}(\xi \dot{\xi}) + \nabla \cdot \left(\frac{\mathbf{j}_e}{T} \right) \\ &= \mathbf{j}_e \cdot \nabla \left(\frac{1}{T} \right) + \frac{1}{T} \text{tr}(\hat{\sigma}^d \dot{\varepsilon}^d) + \frac{1}{T} \text{tr}(\hat{\sigma}^s \dot{\varepsilon}^s) - \rho \text{tr}(\xi^d \dot{\xi}^d) - \rho \text{tr}(\xi^s \dot{\xi}^s) \geq 0. \end{aligned} \quad (5)$$

In the rhs, vectors are present in the first term, scalars in the third and fifth one, and symmetric traceless tensors in the second and fourth term. In an isotropic material, these three types of quantities cannot couple to one another. Therefore, concerning the term containing vectors, we consider Fourier heat conduction, $\mathbf{j}_e = \lambda \nabla \left(\frac{1}{T} \right)$. For the remaining two pairs of terms, the most general Onsagerian solution is

$$\begin{aligned} \hat{\sigma}^d &= l_{11}^d \dot{\varepsilon}^d + l_{12}^d (-\rho T \xi^d), & \hat{\sigma}^s &= l_{11}^s \dot{\varepsilon}^s + l_{12}^s (-\rho T \xi^s), \\ \xi^d &= l_{21}^d \dot{\varepsilon}^d + l_{22}^d (-\rho T \xi^d), & \xi^s &= l_{21}^s \dot{\varepsilon}^s + l_{22}^s (-\rho T \xi^s), \end{aligned} \quad (6)$$

where the $l_{11}^d, l_{12}^d, l_{21}^d, l_{22}^d$ and $l_{11}^s, l_{12}^s, l_{21}^s, l_{22}^s$ material parameters are subjects of thermodynamic restrictions, due to the entropy inequality (5).

Eliminating the internal variable in the constant temperature case also leads to two independent models,

$$\sigma^d + \tau^d \dot{\sigma}^d = E_0^d \varepsilon^d + E_1^d \dot{\varepsilon}^d + E_2^d \ddot{\varepsilon}^d, \quad \sigma^s + \tau^s \dot{\sigma}^s = E_0^s \varepsilon^s + E_1^s \dot{\varepsilon}^s + E_2^s \ddot{\varepsilon}^s, \quad (7)$$

with thermodynamics-originated inequalities for the altogether eight coefficients. The complete model is a deviatoric and a spherical *Kluitenberg–Verhás body*. When $E_2^d = 0$, the deviatoric part reduces to the standard or Poynting–Thomson body of solid rheology. Several simpler rheological bodies may be obtained by a particular choice of the parameters.

A suitable rearrangement reveals the hierarchical structure of the equations:

$$\begin{aligned} (\sigma^d - E_0^d \varepsilon^d) + \tau^d \frac{d}{dt} \left(\sigma^d - \frac{E_1^d}{\tau^d} \varepsilon^d \right) + E_2^d \frac{d^2}{dt^2} \varepsilon^d &= 0, \\ (\sigma^s - E_0^s \varepsilon^s) + \tau^s \frac{d}{dt} \left(\sigma^s - \frac{E_1^s}{\tau^s} \varepsilon^s \right) + E_2^s \frac{d^2}{dt^2} \varepsilon^s &= 0, \end{aligned} \quad (8)$$

In both the deviatoric and the spherical cases, the first term is the pure elastic stress–strain relation, the second is the time derivative of a similar relation with different coefficients and the third one with the highest derivative is an incomplete block, closing the two terms’ hierarchy.

If the coefficients in the consecutive blocks are the same, we may speak about *hierarchical resonance*. If the closure term is zero, a hierarchical resonance may be not dissipative.

In case of specific loading conditions, the deviatoric and spherical parts are coupled but the hierarchical structure may be conserved. It is straightforward to calculate the effective rheological equation in case of uniaxial loading conditions. Denoting the uniaxial stress by $\sigma^||$, one obtains:

$$\sigma^|| - E_0^|| \varepsilon^|| + \tau_1^|| \frac{d}{dt} \left(\sigma^|| - \frac{E_1^||}{\tau_1^||} \varepsilon^|| \right) + \tau_2^|| \frac{d^2}{dt^2} \left(\sigma^|| - \frac{E_2^||}{\tau_2^||} \varepsilon^|| \right) + \tau_3^|| \frac{d^3}{dt^3} \left(\sigma^|| - \frac{E_3^||}{\tau_3^||} \varepsilon^|| \right) + E_4^|| \frac{d^4}{dt^4} \varepsilon^|| = 0 \quad (9)$$

Where $\tau_1^||, \tau_2^||, \tau_3^||$ and $E_0^||, E_1^||, E_2^||, E_3^||$ coefficients are calculated from the spherical and deviatoric coefficients of (7) [8].

In typical experimental situations, the time scales of the different blocks are clearly separated.

3. Hierarchy of wave equations in the theory of dual internal variables

Dual internal variables extend the modeling capability of non-equilibrium thermodynamics by connecting inertial phenomena with dissipation [9]. Dual internal variables coupled to continuum mechanics lead to generalized continua [10, 11]. In this case, the elimination of the internal variables results in a hierarchical structure of wave equations [12, 10, 13].

In what follows, we introduce in brief a one dimensional version of the theory of weakly nonlocal dual internal variables coupled to small-strain elasticity. Therefore, the extended state space is given by the strain, ε , and the internal variables are denoted by ϕ and ξ . In this illustrative example, specific entropy is a quadratic function of the internal variables and their gradients:

$$\tilde{s}(e, \varepsilon, \xi, \phi, \partial_x \xi, \partial_x \phi) = s(e, \varepsilon) - \frac{a_1}{2} \xi^2 - \frac{b_1}{2} (\partial_x \xi)^2 - \frac{a_2}{2} \phi^2 - \frac{b_2}{2} (\partial_x \phi)^2. \quad (10)$$

The Gibbs relation of the weakly nonlocal theory fixes the partial derivatives of the entropy function as

$$\rho d\tilde{s} = \frac{\rho}{T} de - \frac{\sigma}{T} d\varepsilon - \rho a_1 \xi d\xi - \rho a_2 \phi d\phi - \rho b_1 \partial_x \xi d(\partial_x \xi) - \rho b_2 \partial_x \phi d(\partial_x \phi) \quad (11)$$

Assuming the following form of the entropy current density:

$$j_{\tilde{s}} = \frac{q}{T} - \rho \frac{\partial s}{\partial(\partial_x \xi)} \dot{\xi} - \rho \frac{\partial s}{\partial(\partial_x \phi)} \dot{\phi}, \quad (12)$$

one obtains the entropy production similarly to the previous section:

$$T\Sigma = Tq\partial_x \frac{1}{T} + (\sigma - T\rho\partial_\varepsilon s) \dot{\varepsilon} + \underbrace{(\partial_\xi s - \partial_x(\partial_{\partial_x \xi} s))}_{\dot{A}\xi} \dot{\xi} + \underbrace{(\partial_\phi s - \partial_x(\partial_{\partial_x \phi} s))}_{\dot{B}\phi} \dot{\phi} \geq 0. \quad (13)$$

Here, we have introduced a shorthand notation for the internal variable related weakly nonlocal thermodynamic forces. The above form of the entropy current density and entropy production (dissipation inequality) can be also derived with the help of a more detailed thermodynamic analysis, as it has been shown in [11]. Then a linear solution of the above inequality is

$$\begin{aligned}\sigma - E\varepsilon &= l_{11}\dot{\varepsilon} + l_{12}\hat{A}\dot{\xi} + l_{13}\hat{B}\dot{\phi}, \\ \dot{\xi} &= l_{21}\dot{\varepsilon} + l_{22}\hat{A}\dot{\xi} + l_{23}\hat{B}\dot{\phi}, \\ \dot{\phi} &= l_{31}\dot{\varepsilon} + l_{32}\hat{A}\dot{\xi} + l_{33}\hat{B}\dot{\phi}.\end{aligned}\quad (14)$$

In our simple case

$$\hat{A} = -a_1 + b_1\partial_{xx}, \quad \hat{B} = -a_2 + b_2\partial_{xx}.\quad (15)$$

The elimination of the internal variables leads to the following constitutive relation of stress and strain:

$$\begin{aligned}\ddot{\sigma} + (\alpha_1 + \alpha_2\partial_x)\dot{\sigma} + (\beta_1 + \beta_2\partial_x + \beta_3\partial_{xx})\sigma = \\ \ddot{\varepsilon} + (\hat{\alpha}_1 + \hat{\alpha}_2\partial_x)\dot{\varepsilon} + (\hat{\beta}_1 + \hat{\beta}_2\partial_x + \hat{\beta}_3\partial_{xx})\dot{\varepsilon} + (\hat{\gamma}_1 + \hat{\gamma}_2\partial_x + \hat{\gamma}_3\partial_{xx})\varepsilon,\end{aligned}\quad (16)$$

where the coefficients $\alpha_1, \alpha_2, \beta_1, \beta_2, \beta_3$ and $\hat{\alpha}_1, \hat{\alpha}_2, \hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3, \hat{\gamma}_1, \hat{\gamma}_2, \hat{\gamma}_3$ are simple polynomials of the thermodynamic material parameters. The consequence of the momentum balance and the compatibility condition leads to the well-known relation of stress and strain

$$\rho\dot{v} - \partial_x\sigma = 0, \quad \partial_x v = l_1\dot{\varepsilon} \Rightarrow \ddot{\varepsilon} = \partial_{xx}\sigma.\quad (17)$$

Eliminating stress from (16), one obtains the following partial differential equation:

$$\begin{aligned}(\ddot{\varepsilon} - \hat{\alpha}_1\partial_{xx}\dot{\varepsilon}) + (\alpha_1\ddot{\varepsilon} - \hat{\beta}_1\partial_{xx}\dot{\varepsilon}) + (\beta_1\ddot{\varepsilon} - \hat{\gamma}_1\partial_{xx}\dot{\varepsilon}) + \\ \partial_x(\beta_2\ddot{\varepsilon} - \hat{\gamma}_2\partial_{xx}\dot{\varepsilon}) + \partial_{xx}(\beta_3\ddot{\varepsilon} - \hat{\gamma}_3\partial_{xx}\dot{\varepsilon}) - \partial_{xx}(l_1\ddot{\varepsilon} + \hat{\beta}_3\partial_{xx}\dot{\varepsilon} + \alpha_2\partial_x\dot{\varepsilon}) = 0.\end{aligned}\quad (18)$$

Mixed space and time derivatives of coupled wave equations are analysed in detail and are compared to various wave propagation models in [13].

4. Hierarchy of Fourier equations and generalized heat conduction with current multipliers

Non-equilibrium thermodynamics with current multipliers introduces a unified constitutive theory of heat conduction where several generalizations of Fourier equation may be obtained as special cases [14]. Moreover, it is shown that the structure is compatible with the moment series expansion of kinetic theory, at least up to the third moment [15]. In this framework, the basic state space is extended by the heat flux \mathbf{q} and also by a second order tensorial internal variable \mathbf{Q} . We assume the usual quadratic form of the entropy function at the extended part of the state space,

$$\tilde{s}(e, \mathbf{q}, \mathbf{Q}) = s(e) - \frac{m_1}{2}\mathbf{q}^2 - \frac{m_2}{2}\mathbf{Q}^2.\quad (19)$$

Then a generalized entropy current is introduced in the following form:

$$\mathbf{j}_q = \mathbf{b} \cdot \mathbf{q} + \mathbf{B} : \mathbf{Q}.\quad (20)$$

Here, the current multipliers \mathbf{b} and \mathbf{B} are second and third order tensors, respectively. This form of the generalized entropy current was introduced by Nyíri [16]. \mathbf{b} and \mathbf{B} are to be determined as constitutive functions with the help of the entropy inequality. A short calculation results in

$$\Sigma = \left(\mathbf{b} - \frac{1}{T}\mathbf{I} \right) : \nabla \mathbf{q} - (\nabla \mathbf{b} - m_1\dot{\mathbf{q}}) \cdot \mathbf{q} - (\nabla \cdot \mathbf{B} - m_2\dot{\mathbf{Q}}) : \mathbf{Q} + \mathbf{B} : \nabla \mathbf{Q} \geq 0.\quad (21)$$

Here the number of the central dots denotes one, two and three contractions of the first, second and third order tensors, respectively. The first and the third terms are products of second order tensors, the second term is vectorial, and the last term is a product of third order tensors. Therefore, for isotropic materials, cross effects may appear only between the first and the third terms. Hence, in a one dimensional simplification, linear relations between the thermodynamic fluxes and forces are as follows:

$$m_1 \dot{q} - \partial_x b = -l_1 q, \quad (22)$$

$$m_2 \dot{Q} - \partial_x B = -k_1 Q + k_{12} \partial_x q, \quad (23)$$

$$b - \frac{1}{T} = -k_{21} Q + k_2 \partial_x q, \quad (24)$$

$$B = n_3 \partial_x Q, \quad (25)$$

where ∂_x denotes the one dimensional spatial derivative and the material coefficients $m_1, m_2, l_1, k_1, k_2, k_{12}, k_{21}, n_3$ are subjects to thermodynamical constraints. It is straightforward to eliminate the current multipliers and the tensorial internal variable Q . Then one obtains the following equation:

$$m_1 m_2 \ddot{q} + (m_2 l_1 + m_1 k_1) \dot{q} - (m_2 k_2 + m_1 n_3) \partial_{xx} \dot{q} + k_1 l_1 q - (k_1 k_2 - k_{12} k_{21} + l_1 n_3) \partial_{xx} q + k_2 n_3 \partial_{xxx} q - k_1 \partial_{xt} \left(\frac{1}{T} \right) - m_2 \partial_x \left(\frac{1}{T} \right) + m_3 \partial_{xxx} \left(\frac{1}{T} \right) = 0 \quad (26)$$

In our case, the balance of internal energy (4) is

$$\rho c \dot{T} + \partial_x q = 0, \quad (27)$$

where ρ is the density and c is the specific heat. The combination of (26) and (27) may be written in the following form:

$$\begin{aligned} & \left((m_2 l_1 + m_1 k_1) \dot{T} - \frac{m_2}{\rho c T^2} \partial_{xx} T \right) + k_1 \left(l_1 \dot{T} - \frac{1}{\rho c T^2} \partial_{xx} T \right) + \\ & \partial_{xx} \left((k_1 k_2 - k_{12} k_{21} + l_1 n_3) \dot{T} - \frac{n_3}{\rho c T^2} \partial_{xx} T \right) + \\ & (m_2 m_1 \dot{T} - (m_1 n_3 + m_2 k_2) \partial_{xx} T) + k_2 n_3 \partial_{xxx} T = 0. \end{aligned} \quad (28)$$

We can observe various time and space derivatives of the Fourier equation in different forms, plus the last term with the highest derivatives. The arrangement is space-time hierarchical, like in the previous section.

4.1. Hierarchical resonance: the example of the Guyer–Krumhansl equation

The hierarchical rearrangement of an evolution equation may help in recognizing solution patterns. In this subsection, we give a simple example with the help of the Guyer–Krumhansl equation.

The Guyer–Krumhansl equation is obtained when $n_3 = k_2 = m_1 = k_{12} = 0$ in (28):

$$\tau_q \partial_t \left(\partial_t T - \frac{a}{\tau_q} \partial_{xx} T \right) + \partial_t T - \lambda \partial_{xx} T = 0. \quad (29)$$

Here, $\tau_q = m_2/k_1$, $\lambda = 1/(\rho c k_1 l_1 T^2)$ and $a = m_2/(\rho c k_1 l_1)$, and these coefficients are considered constant. This is a two-level hierarchical arrangement. If $\tau_q = 0$ then the first term is zero, and the hierarchy is reduced to a single Fourier equation. If $a = \tau_q \lambda$ then there appears the same Fourier equation in both terms. This is the case of *hierarchical resonance* [15] and the solutions of the coupled set of equations may be identical to the single Fourier equation.

The resonance may help to classify the solutions. Let us introduce adiabatic boundary at the end of a rod and heat pulse boundary conditions at the the front side in the following form:

$$q_0(t) = q(x=0, t) = \begin{cases} q_{\max} \left(1 - \cos \left(2\pi \cdot \frac{t}{t_p} \right) \right) & \text{if } 0 < t \leq t_p, \\ 0 & \text{if } t > t_p. \end{cases}$$

Here t_p is the duration of the pulse and q_{\max} is the maximum of the heat flux at the boundary. Initially, the temperature is uniform and there is no heat flux $q(t=0, x) = 0$, $T(t=0, x) = T_0$. Then the solutions show characteristic differences depending on whether the parameters are above or below the resonance value. This is represented on Figure 1, where temperature and time are the following dimensionless quantities: $\hat{t} = \frac{\lambda t}{\rho c L^2}$ and $\hat{T} = \frac{T - T_0}{T_{\text{end}} - T_0}$. Here L is the length of the rod and T_{end} is the asymptotic value of the temperature after the equilibration.

- If $a = \tau_q \lambda$ then we obtain the solution of the Fourier equation. This is the solid line on Fig. 1.
- If $a < \tau_q \lambda$ then we obtain solutions where temperature starts to increase later than in the Fourier solution. For short rods, the heat pulse is observable. The important characteristics of the solution are similar the solutions of the Maxwell–Cattaneo–Vernotte equation. This is the dashed line on Fig. 1.
- If $a > \tau_q \lambda$ then temperature starts to increase earlier than for the Fourier solution. The remnants of the heat pulse are not observable, and sometimes there is a change in the steepness of the solution, a kink. The solution is more damped than the Fourier one. This is the dashed-dotted line on Fig. 1.

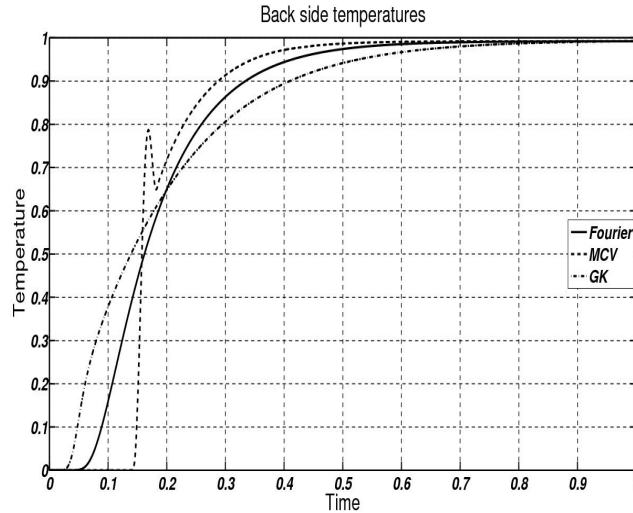


Fig. 1. Characteristic solutions of the Guyer–Krumhansl equation in case of heat pulse experiments.

5. Summary

Eliminating internal variables in non-equilibrium thermodynamics results in a hierarchical structure of the evolution equation. The building block of the hierarchy is the evolution equation of the original theory, which was supplemented by the internal variable.

The solution of the original equation may appear at different particular values of the parameters. If this happens with more than one nonzero elements of the hierarchy, we can call it hierarchical resonance.

6. Acknowledgement

The work was supported by the grants OTKA K81161 and K104260.

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